

3-Methyl-1-nitrobutane
627-67-8 | DTXSID90211769

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.74

Global applicability domain: Inside

Local applicability domain index: 6.63e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

Image not found

1-Nitropentane

Measured: 2.01

Predicted: 1.83

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Propane, 2-methyl-2-nitro-

Measured: 1.17

Predicted: 1.33

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Propane, 2-methyl-1-nitro-

Measured: 1.40

Predicted: 1.42

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1-Nitrohexane

Measured: 2.70

Predicted: 2.24

Image not found

1-Nitrobutane

Measured: 1.47

Predicted: 1.35